Role of the H Theorem in Lattice Boltzmann Hydrodynamic Simulations

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In the last decade, minimal kinetic models, and primarily the Lattice Boltmann equation, have met with significant success in the simulation of complex hydrodynamic phenomena, ranging from slow flows in grossly irregular geometries to fully developed turbulence, to flows with dynamic phase transitions. Besides their practical value as efficient computational tools for the dynamics complex systems, these minimal models may also represent a new conceptual paradigm in modern computational statistical mechanics: instead of proceeding bottom-up from the underlying micro-dynamic systems, these minimal kinetic models are built top-down starting from the macroscopic target equations. This procedure can provide dramatic advantages, provided the essential physics is not lost along the way. For dissipative systems, one such essential requirement is the compliance with the Second Law of thermodynamics.

In this Colloquium, we present a chronological survey of the main ideas behind the Lattice Boltzmann method, with special focus on the role played by the H theorem in enforcing compliance of the method with macroscopic evolutionary constraints (Second Law) as well as in serving as a numerically stable computational tool for fluid flows and other dissipative systems out of equilibrium.

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I. INTRODUCTION

The quest for a better understanding of the macroscopic world in terms of underlying "fundamental" microscopic laws is a timeless issue in the history of science and natural philosophy. Modern science has provided an admirably powerful theory, and mathematical tool as well, to address this issue in a sensible and productive way, a gift named Newtonian mechanics. Newtonian mechanics is a theory of amazing depth and breadth, going as it does from scales of planetary motion, all the way down to molecular trajectories, encompassing almost *twenty orders of magnitude* in the process.

Besides an array of practical results, the application of Newtonian mechanics at the molecular scale generates a profound puzzle: the origin of *irreversibility* and the nature of time itself. Newton's equations are manifestly reversible, that is, invariant under time and velocity inversion, which means that molecular motion is basically like a movie which can be indifferently rolled forwards or backwards in time with no loss of information. This is in blatant contrast to our daily experience of an inexorably one-sided nature of time evolution: the arrow of time travels only one-way. This puzzle has remained

outstanding for more than a century, and is still open to a large extent, and in any case is beyond the scope of the present work. Besides its profound philosophical implications, irreversibility also bears upon the practical question of predicting the macroscopic behaviour of complex systems comprising a huge number of (non-linearly) interacting individual units. The application of Newtonian mechanics to the molecular scale inevitably leads to a gigantic wave of *computational complexity* due to the enormous number of atoms/molecules constituting macroscopic systems. This problem is circumvented by formulating *continuum* models, typically based on partial differential equations describing the space-time evolution of a few macroscopic fields, such as fluid density, pressure, temperature, and so on. This approach is indeed quite successful, but when confronted with complex systems out of equilibrium, e.g., fully turbulent flows, it shows clear limitations. The point is that, owing to strong non-linearities and multi-dimensionality, the aforementioned partial differential equations are often just too complicated to be solved by even the most powerful numerical techniques. It therefore makes sense to go back to Newtonian-like dynamics, namely large sets of *ordinary* differential equations, and develop *minimal* fictitious particle dynamics designed so as to relinquish as many microscopic details as possible without corrupting the ultimate macroscopic target.

In this work, we shall be concerned precisely with this type of modelling strategy. In particular, we shall turn our attention to alternative ways to gain understanding about the *predictability* of macroscopic phenomena out of hyperstylized "Newton-like" microscopic *models*. We hasten to add that these alternative routes are highly influenced by advances in computational modelling, and therefore they naturally fit into the general framework of computational statistical mechanics. Like their real-life physical counterparts, these hyperstylized models are required to display irreversible behaviour as a basic requisite of stability, whence the importance of designing them in compliance with the second law of thermodynamics. In this Colloquium we shall be concerned with the Lattice Boltzmann equation, a minimal form of the Boltzmann equation which retains just the least amount of kinetic information neeeded to recover correct hydrodynamics as a macroscopic limit. The Lattice Boltzmann equation has proved quite effective in describing a variety of complex flow situations using a very simple and elegant formalism built upon the aforementioned hyperstylized approach.

II. STATISTICAL MECHANICS BACKGROUND

The theory of the Lattice Boltzmann equation belongs to the general framework of non-equilibrium statistical mechanics. In this section we shall therefore present a brief review of the main cornerstones of classical statistical mechanics, starting from the most fundamental

(atomistic) level, all the way up to the macroscopic level.

For most practical purposes, our ability to predict the behaviour of the world around us depends upon the time evolution of macroscopic variables, e.g., pressure, temperature, flow speedsr, etc., which result from the collective average over of an enormous amount of individual trajectories. Since we can only experience average quantities, it makes sense to think of mathematical formulations dealing directly with these average quantities: which is the chief task of Statistical Mechanics.

A. The BBGKY hierarchy

The traditional route to this end is the celebrated BBGKY (Bogoliubov-Born-Green-Kirkwood-Yvon) hierarchy (Cercignani, 1975, Liboff, 1998), leading from atomistic equations to fluid dynamic equations for the macroscopic variables, typically the Navier-Stokes equation of fluid flow (Landau and Lifshitz, 1953).

The BBGKY path is based on the four basic levels (see left branch of Figure 1):

- *Atomistic level (Newton-Hamilton)*
- *Many-body kinetic level (Liouville)*
- *One-body kinetic level (Boltzmann)*
- *Macroscopic level (Navier-Stokes)*

Let us discuss these four levels is some more detail.

B. The atomistic level

The atomistic description of (classical) macroscopic systems is based on Newtonian mechanics. The mathematical problem generated by Newtonian mechanics is to solve a set of N non-linear ordinary differential equations:

$$m_i \frac{d^2 \boldsymbol{x}_i}{dt^2} = \boldsymbol{F}_i, \tag{1}$$

with the initial conditions:

$$\boldsymbol{x}_i(t=0) = \boldsymbol{x}_{0i} \tag{2}$$
$$\boldsymbol{v}_i(t=0) = \boldsymbol{v}_{0i}, \quad i = 1, N$$

where N is of the order of Avogadro's number $N_A \sim 6 \times 10^{23}$. In the above, m_i are the molecular masses, $\boldsymbol{v}_i = d\boldsymbol{x}_i/dt$ the molecular speeds and $\boldsymbol{F}_i$ is the force acting upon the i-th molecule due to intermolecular interactions (Huang, 1987).

The application of Newtonian mechanics to the molecular world prompts a daunting wave of *computational complexity*. A centimeter cube of an ordinary substance, say water, contains of the order of Avogadro's number of molecules. Keeping track of the motion of these many molecules in the way portrayed by Laplace, namely by

tracing in time the $6N$ variables $\boldsymbol{x}_i(t)$ and $\boldsymbol{v}_i(t)$ turns out to be a scientific *chimera*. Even assuming one has enough capacity to store so much information, one would still be left with the problem of dynamic instabilities in phase space: any tiny uncertainty in the initial microscopic state would blow up exponentially in time, thereby shrinking the predictability horizon of the system virtually to zero. It is a great gift that such a huge amount of information, besides being unmanageable, is also needless as well, as we shall see in the next section.

C. Many-body kinetic level

The atomistic level deals with molecular positions and speeds and is governed by the Newton-Hamilton equations which describe a world of *trajectories*. The N-body kinetic level deals with *distribution functions* $f_N(\boldsymbol{x}_1, \boldsymbol{v}_1 \ldots \boldsymbol{x}_N, \boldsymbol{v}_N, t)$, namely smooth fields describing the joint probability to find molecule 1 at position $\boldsymbol{x}_1$ with speed $\boldsymbol{v}_1$, *and* molecule 2 at position x_2 with speed $\boldsymbol{v}_2$, and so on up to molecule N around position $\boldsymbol{x}_N$ with speed $\boldsymbol{v}_N$, all at the same time t. Trajectories are here replaced by the notion of *phase-space* fluids obeying a $6N$ dimensional continuity equation, known as the *Liouville equation*:

$$[\partial_t + \sum_{i=1}^{N} \boldsymbol{v}_i \cdot \partial_{\boldsymbol{x}_i} + \boldsymbol{a}_i \cdot \partial_{\boldsymbol{v}_i}]f_N = 0 \qquad (3)$$

where $\boldsymbol{a}_i = \boldsymbol{F}_i/m_i$ are the molecular accelerations. The underlying assumption is *ergodicity*: the time spent by the trajectory of the $6N$ dimensional coordinate $P(t) \equiv [\boldsymbol{x}_1(t) \ldots \boldsymbol{v}_N(t)]$ in a given differential volume element $\Delta\Gamma$ of phase space, is proportional to the measure of $\Delta\Gamma$.

The Liouville equation does not *by any means* reduce the amount of information to be handled via the Newtonian approach. In fact, since f_N is a continuum $6N$ dimensional field, the amount of *computational* information blows up exponentially! The Liouville equation represents nonetheless a very valuable step, not because we can solve it, but because it sets the stage for a very elegant and powerful procedure to consistently eliminate irrelevant information. Simply integrate f_N over unwanted single-particle coordinates, to define low-order reduced distribution functions $f_M \equiv f_{12\ldots M<N} = \int f_{12\ldots N} dz_{M+1}\ldots dz_N$, where $dz_k \equiv dx_k dv_k$, $k = M+1, \ldots N$. The result is a chain of equations:

$$[\partial_t + \sum_{i=1}^{M} \boldsymbol{v}_i \cdot \partial_{\boldsymbol{x}_i} + \boldsymbol{a}_i \cdot \partial_{\boldsymbol{v}_i}]f_M = C_M \qquad (4)$$

known as the BBGKY hierarchy. Note that the right-hand side collects the effects of intermolecular interactions. In the presence of a b-body potential, C_M only involves b upper-lying distributions $f_{M+1}, \ldots f_{M+b}$. Fortunately, most interesting macroscopic observables, such as density, pressure, temperature, and energy, only depend on 1 or 2-body distributions, so that our efforts can

be channeled into the bottom floors, $M = 1, 2$, of the BBGKY hierarchy.

D. The Boltzmann equation and the H-theorem

The most important one-body equation is the celebrated Boltzmann equation:

$$\partial_t f + \boldsymbol{v} \cdot \partial_{\boldsymbol{x}} f + \boldsymbol{a} \cdot \partial_{\boldsymbol{v}} f = C[f, f] \qquad (5)$$

where $f(\boldsymbol{x}, \boldsymbol{v}, t)$ is the probability density of finding a classical pointlike particle at position $\boldsymbol{x}$ at time t with speed $\boldsymbol{v}$. The left hand side represents free streaming in phase space $(\boldsymbol{x}, \boldsymbol{v})$ and the right hand side denotes the effects of binary collisions, typically a very complicated integral operator encoding the details of molecular interactions. The Boltzmann equation relies on the famous molecular chaos (*"Stosszahlansatz"*) assumption:

$$f_{12}(\boldsymbol{x}_1, \boldsymbol{v}_1, \boldsymbol{x}_2, \boldsymbol{v}_2, t) = f(\boldsymbol{x}_1, \boldsymbol{v}_1, t)f(\boldsymbol{x}_2, \boldsymbol{v}_2, t) \quad (6)$$

which asserts the absence of correlations between molecules entering a binary collision. It is precisely this arbitrary–if plausible– assumption which breaks time-reversal symmetry, since it is clear that *after* a collision molecules must be correlated because of mass-momentum-energy conservation. The essence of the molecular chaos assumption is that these post-collisional correlations decay exponentially fast in time so that the probability of the two particles to collide with each other again in a correlated state after any finite time lapse is virtually zero. Breaking time-reversal symmetry opens the door to irreversible behavior, and one of the most profound of Boltzmann's contributions to statistical mechanics rests with his discovery of a quantitative measure of irreversibility: the celebrated H-theorem. This quantitative measure of irreversibility is provided by the Boltzmann H-function (in what follows, we term it also as the entropy function; the physical entropy being $S = -k_{\mathrm{B}}H$):

$$H(t) = \int f(\boldsymbol{x}, \boldsymbol{v}, t) \ln f(\boldsymbol{x}, \boldsymbol{v}, t) d\boldsymbol{v} d\boldsymbol{x} \qquad (7)$$

which was shown by Boltzmann to be monotonically non-increasing in time, $dH/dt \leq 0$, *regardless* of the details of the collision operator. The H-theorem stands out as a conceptual bridge between micro- and macro-dynamics. Yet, it is difficult to think of a more debated and controversial issue in theoretical physics (see Wehrl, 1978). We will not delve here into the details of the various paradoxes which were raised against the H-theorem, nor shall we discuss the fact that Boltzmann derived his theorem without demonstrating under which conditions his equation, a complicated integro-differential initial-value problem, does indeed have solutions. While leaving mathematical rigor somehow behind, the H-theorem is nonetheless a monumental contribution to modern science, since it showed for the first time the way to a grand-unification of two fundamental and hitherto disconnected domains of science: Mechanics and Thermodynamics.

The practical importance of Boltzmann-like equations was only to be furthered by modern developments in theoretical physics, primarily the emergence of the fundamental notion of *quasi-particles* as collective excitations of non-linear field theories (Kadanoff and Baym, 1962). By shifting the focus from actual particles (real atoms or molecules) to quasi-particles, the Boltzmann equation goes way beyond the original framework from which it was derived (i.e., rarefied gas dynamics) and spreads nowadays its wings across a huge variety of fields in statistical mechanics, including neutron and radiation transport, electron transport in semiconductors, hadronic plasmas, and many others. Quasi-particles play a central role also in the top-down approach to statistical mechanics that is to be described shortly.

E. The macroscopic level

Macroscopic observables such as fluid mass density, speed and energy density are obtained from the one-body kinetic distribution by integration over velocity space:

$$\rho(\boldsymbol{x},t) = m \int f(\boldsymbol{x},\boldsymbol{v},t)d\boldsymbol{v}, \qquad (8)$$

$$\rho\boldsymbol{u}(\boldsymbol{x},t) = m \int f(\boldsymbol{x},\boldsymbol{v},t)\boldsymbol{v}d\boldsymbol{v},$$

$$\rho e(\boldsymbol{x},t) = m \int f(\boldsymbol{x},\boldsymbol{v},t)\frac{v^2}{2}d\boldsymbol{v}$$

where m is the atomic/molecular mass. Supplementing these formal integrations with additional assumptions (e.g., small deviations from local thermodynamic equilibrium), one finally arrives at the desired equations for the macroscopic observables, typically the Navier Stokes equations of fluid dynamics (for the time being, we restrict ourselves to the case of isothermal fluids, for which the energy equation is not needed):

$$\partial_t\rho + \mathrm{div}(\rho\boldsymbol{u}) = 0, \quad (9)$$
$$\partial_t\rho\boldsymbol{u} + \mathrm{div}(\rho\boldsymbol{u}\boldsymbol{u}) = -\nabla P + \mathrm{div}(2\mu\overline{\nabla\boldsymbol{u}} + \lambda\mathbf{1}\mathrm{div}\boldsymbol{u}),$$

where ρ is the fluid density, $\boldsymbol{u}$ the fluid speed, P the fluid pressure, the overline denotes the symmetric dyad $\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^T$, the superscript T indicates the transpose, μ and λ are the shear and bulk dynamic viscosities respectively, and $\mathbf{1}$ denotes the tensor identity. The Navier-Stokes equations keep no track of the discrete nature of the underlying microscopic world, and are paramount for the quantitative description of macroscopic systems.

F. The top-down approach

Each jump down the BBGKY ladder removes irrelevant information so that, in the end, the 10^{23} atomistic trajectories are replaced by the evolution of a handful of continuum hydrodynamic fields.

The BBGKY approach is formally elegant and very fruitful for further theoretical insight and analysis. In fact, it is perfectly positioned to borrow the powerful mathematical machinery of classical and quantum statistical field theory, such as perturbative methods, diagrammatic techniques and the like. Less noted, perhaps, is the fact that the resulting equations prove *exceedingly difficult* to solve in actual practice. This is true even at the coarsest level: the Navier-Stokes equations are notorious for posing one of the hardest problems left in classical (i.e., non quantum) physics, namely fluid turbulence. It makes sense therefore to think of complementary routes to BBGKY, more aligned with the spirit of model-building and computational tractability rather than with amenability to analytical treatment.

An emerging and still fast-developing strategy along these lines is provided by *fictitious dynamics* methods. The idea is to introduce effective molecules (*"computational quasi-particles"*), each representing a huge number, say R, of real ones, so that the number of effective molecules we must deal with is no longer of the order of Avogadro's number, but of order $N_R = N_A/R << N_A$ instead. In terms of these effective molecules, the Newtonian equations are as follows:

$$M_I\frac{d^2\boldsymbol{X}_I}{dt^2} = \boldsymbol{F}_I(\boldsymbol{X}) + \boldsymbol{D}_I, \quad I = 1, N_R \qquad (10)$$

where $\boldsymbol{X}_I$ represents a coarse-grained coordinate, and $M_I = \sum_{i=1}^R m_i$ is the total mass of the effective "macromolecule". The term $\boldsymbol{D}_I$ collects all the details of the underlying fine-scales and disappears only in the trivial case of a linear dependence of the force $\boldsymbol{F}_I$ on the molecular coordinates. Realistic forces are generally inverse powers of the intermolecular distance and, consequently, $\boldsymbol{D}_I \neq 0$. A proper renormalization/closure procedure would attempt to incorporate the effects of the fine scales into appropriate (and most likely very complicated) expressions for a renormalized force $\tilde{\boldsymbol{F}}_I = \boldsymbol{F}_I + \hat{C}\boldsymbol{D}_I$, $\hat{C}$ being some form of projection operator making the renormalized force available in terms of the coarse-grained coordinates. Most simply, one sets $\boldsymbol{D}_I = 0$ and proceeds with the solution of the *same* Newtonian equations, only applied to a much smaller set of molecules: this is the very successful path taken by Molecular Dynamics (Alder and Wainwright, 1959).

However, once it is agreed that the ultimate aim is macroscopic physics, say solving the Navier-Stokes equations, even Molecular Dynamics is still redundant of needless micro-details. We may want more than just setting $\boldsymbol{D}_I = 0$, and look for instance for expressions of the coarse-grained force $\tilde{\boldsymbol{F}}_I$ that are simpler than those associated with true intermolecular interactions. The principle of Occam's razor, i.e., maximum simplicity implies that one should choose the simplest coarse-grained dynamics compatible with the target macroscopic equations. This is the hard-core idea of "minimal molecular dynamics": relinquish as many microscopic details as possible right at the outset (atomistic level), making sure,

however, that the basic symmetries, conservation laws and evolutionary constraints needed to ensure the correct macroscopic behaviour are preserved in the process. As to the first principle of thermodynamics, this means conserving all-and only-the microscopic invariants (mass, momentum, energy), while compliance with the second principle of thermodynamics imposes the existence of a suitable monotonically increasing function of time, the Boltzmann H-function and the related entropy. The actual realization of the top-down approach is by no means unique (for a recent form of dissipative particle dynamics, see Hoogerbrugge and Koelman, 1992, Espanol and Warren, 1995, Flekkoy and Coveney, 1999). In the following, however, we shall refer to Lattice Gas Cellular Automata (LGCA), a particularly appealing instance of minimal particle dynamics developed in the mid 1980's, which provided the roots of the Lattice Boltzmann (LB) method.

III. LATTICE GAS CELLULAR AUTOMATA

The theory of lattice Gas Cellular Automata is a rich subject and has been recently made accessible in full detail by a series of beautiful monographs (Rothman and Zaleski, 1997, Chopard and Droz, 1998, Rivet and Boon, 2001). Here we shall take a substantial shortcut and proceed by example.

A. The Frisch-Hasslacher-Pomeau automaton

Let us begin by considering a regular lattice with hexagonal symmetry such that each lattice site is surrounded by six neighbors identified by six connecting speeds $\boldsymbol{v}_i \equiv v_{ia}$, $i = 1, 6$, the index $a = 1, 2$ running over the spatial dimensions x, y (see Figure 2, which also includes a rest-particle with zero speed). Each lattice site hosts up to six particles with the following prescriptions

- All particles have the same mass $m = 1$

- Particles can move only along one of the six directions defined by the discrete displacements v_{ia}.

- In a time-cycle (set at unity for convenience) the particles hop synchronously to the nearest neighbor in the direction of the corresponding discrete vector v_{ia}. Longer or shorter jumps are both forbidden, which means all lattice particles have the same energy.

- No two particles sitting on the same site can move along the same direction v_{ia} (*Exclusion Principle*).

These prescriptions identify a very stylized gas analogue, whose dynamics is made purposely unaware of microscopic details of real-molecule Newtonian dynamics. In a real gas molecules move along any direction (*isotropy*) whereas here they are confined to a hexagonal cage. Also,

real molecules can move virtually at any (subluminal) speed, whereas here only six mono-energetic beams are allowed. Amazingly, this apparently poor representation of true molecular dynamics has all it takes to simulate realistic hydrodynamics! With the prescription kit given above, the state of the system at each lattice site is unambiguously specified in terms of a plain *yes/no* option saying whether or not a particle sits on the given site. This dichotomic situation is readily coded with a single binary-digit (bit) per site and direction so that the entire state of the lattice gas is specified by $6N$ bits, N being the number of lattice sites. Borrowing the parlance of second quantization, we introduce an *occupation number* n_i, such that

$$ n_i(\boldsymbol{x}, t) = \{1, 0\} \tag{11} $$

depending on whether or not the lattice site $\boldsymbol{x}$ hosts a particle with speed $\boldsymbol{v}_i$ at time t. The collection of occupation numbers $n_i(\boldsymbol{x}, t)$ over the entire lattice defines a $6N$ dimensional time-dependent boolean field whose evolution takes place in a boolean phase-space consisting of 2^{6N} discrete states. This boolean field takes the intriguing name of *Cellular Automaton* to emphasize the idea that not only space and time, but also the dependent variables (matter) take on discrete (boolean) values. The fine-grain microdynamics of this boolean field *cannot* be expected to reproduce the true molecular dynamics to any reasonable degree of microscopic accuracy. However, as is known since Gibbs, many different microscopic systems can give rise to the same macroscopic dynamics, and it can therefore be hoped that the macroscopic dynamics of the lattice boolean field would replicate real-life hydrodynamic motion even if its microdynamics does not.

B. Boolean microdynamics

Let us now prescribe the evolution rules of our cellular automaton. Since we aim at hydrodynamics, we should address two basic mechanisms:
- *Free-streaming*
- *Collisions*

Free streaming consists of simple particle transfers from site to site with discrete speeds $\boldsymbol{v}_i$. Thus, a particle sitting at site $\boldsymbol{x}$ at time t with speed v_{ia} will move to site $\boldsymbol{x} + \boldsymbol{v}_i$ at time $t + 1$.

In equations:

$$ n_i(\boldsymbol{x} + \boldsymbol{v}_i, t + 1) = n_i(\boldsymbol{x}, t) \tag{12} $$

This defines the discrete free-streaming operator S_i as

$$ S_i n_i \equiv n_i(\boldsymbol{x} + \boldsymbol{v}_i, t + 1) - n_i(\boldsymbol{x}, t) \tag{13} $$

This operator is a direct transcription of the Boltzmann free-streaming operator, $D_t \equiv \partial_t + v_a \partial_a$, to a discrete lattice in which space-time variables are discretized according to the synchronous "light-cone" rule:

$$\Delta x_{ia} = v_{ia}\Delta t. \tag{14}$$

Once on the same site, particles interact and reshuffle their momenta so as to exchange mass and momentum among the different directions allowed by the lattice (see Figure 3).

This mimics the real-life collisions taking place in a real gas, with the crude restriction that all pre- and post-collisional momenta are forced to "live" on the lattice. As compared with continuum kinetic theory, Lattice Gas Cellular Automata introduces a very radical cut of degrees of freedom in momentum space: just one speed (all discrete speeds share the same magnitude $c = 1$, hence the same energy) and only six different propagation angles. Not bad for an original set of six-fold infinite degrees of freedom! Space-time is also discretized (see (14)), but this is common to all computer simulations of dynamical systems. At this stage, it is still hard to believe that such a stylized system can display all of the complexities of fluid phenomena. And yet it does! The reader acquainted with modern statistical mechanics smells the sweet scent of *universality*: for all its simplicity, the Frisch-Hasslacher-Pomeau automaton may display the same large-scale properties of a real fluid (Kadanoff, 1986), such as propagation of sound waves, vortex interactions and energy dissipation. The name of this magic is *symmetry and conservation*.

Let us dig a bit deeper into this matter.

Let us consider the Frisch-Hasslacher-Pomeau collision depicted in Figure 3: Albeit stylized, this collision shares two crucial features with a real molecular collision:

- It conserves particle number (2 before, 2 after)

- It conserves total momentum (0 before, 0 after)

Symbolically, its effect on the occupation numbers is a change from n_i to n_i' on the same site

$$n_i' - n_i = C_i(\underline{n}) \tag{15}$$

where $\underline{n} \equiv [n_1, n_2 \ldots n_b]$ denotes the set of occupation numbers at a given lattice site.

To sum up, the final Lattice Gas Cellular Automata update rule reads as follows:

$$S_i n_i = C_i \tag{16}$$

or, which is the same:

$$n_i(\boldsymbol{x} + \boldsymbol{v}_i, t+1) = n_i'(\boldsymbol{x}, t) \tag{17}$$

where all quantities have been defined previously. The equations (16, 17) represent the microdynamic equation for the boolean lattice gas, the analogue of Newton equations for real molecules. This equation constitutes the starting point of a Lattice BBGKY hierarchy, ending up with the Navier-Stokes equations. At each level, one formulates a lattice counterpart of the various approximations pertaining to the four levels of the hierarchy (see Figure 1).

C. Merits and pitfalls of Lattice Gas Automata

The major appeals of Lattice Gas Cellular Automata are:

- *Round-off free computing (boolean algebra is exact)*

- *Memory savings (only one bit per degree of freedom)*

- *Virtually unlimited potential for parallel computing*

These points fueled the excitment around Lattice Gas Cellular Automata as a potentially revolutionary tool for computational fluid dynamics (and more). In particular, the hope was to attack the infamous problem of fluid turbulence. Let us just mention that this relates to the dynamics of flows where dissipative effects are very small as compared with advection. The relative strength of advection versus dissipation is measured by a dimensionless number known as the Reynolds number:

$$Re = \frac{UL}{\nu} \tag{18}$$

where U is a typical flow speed on a macroscopic scale L (the size of the device) and ν is the kinematic viscosity of the fluid. Based on dimensional scaling theories (A.N. Kolmogorov, 1941), it can be shown that the number of degrees of freedom associated with a turbulent flow at a given Reynolds number Re is approximately $Re^{9/4}$. Since $Re \sim 10^6$ is a commonplace in daily life (that's more or less what we experience by driving our car at cruising speed of about 100 Km/h in full compliance with traffic regulations...), the simulation of such flows implies the solution of about 10^{14} degrees of freedom: less than Avogadro's number, to be sure, but still too much for any foreseeable computer. These figures say it all as to the hunger for innovative mathematical and numerical methods for fluid turbulence! Unfortunately, closer inspection into the details of the Lattice Gas Cellular Automata method reveal a number of difficult problems:

- *Statistical noise*

- *Complexity of the collision operator*

- *Small number of collisions*

Statistical noise relates to the fact that in order to extract a smooth hydrodynamic signal, averages over *many* boolean variables are required, thereby eclipsing the memory savings provided by the boolean microdynamic representation.

Exponential complexity relates to the exponential escalation of the collision operator as more physics is added to the model, say, more than one fluid species, or simply by moving to higher dimensions. The problem is that the complexity of the corresponding collision operator grows exponentially, roughly as 2^b, where b is the number of bits per site, so that the original simplicity is rapidly lost.

Low collisionality is also related to the paucity of discrete speeds. Only a relatively small fraction of phase space is collisionally active since many collisions are simply not compatible with conservation principles. Few collisions mean long mean-free-path, hence high momentum diffusivity ν, hence low-Reynolds numbers, and the dream of simulating highly turbulent flows fades away.

In spite of the remarkable progresses achieved in the late 1980's, the Lattice Gas Cellular Automata algorithms remained rather heavy and stiff with respect to the collision rules. On the other hand, these inconveniences were not compensated by a dramatic advantage in terms of accessible Reynolds numbers. As a result, the interest in Lattice Gas Cellular Automata as a tool for high Reynolds flow simulations leveled off in the early 1990's. This was precisely the time the Lattice Boltzmann method took off.

IV. LATTICE BOLTZMANN EQUATIONS

The theory of the lattice Boltzmann equation (LBE) (for a review see, Benzi, Succi, Vegassola, 1992, Qian, Succi, Orszag, 1995 and Chen, Doolen, 1998) begins with a straightforward floating point recast of the boolean evolution equation of Lattice Gas Cellular Automata dynamics (Frisch, Hasslacher and Pomeau, 1986; Frisch *et al.*, 1987). With reference to a set of b populations, $f_i(\boldsymbol{x}, t)$, with $\{i = 1, \ldots, b\}$ representing the probability for a particle to reside on a lattice site $\boldsymbol{x}$ at time t with discrete velocity $\boldsymbol{v}_i$, the LBE reads as follows:

$$f_i(\boldsymbol{x} + \boldsymbol{v}_i, t+1) = f_i(\boldsymbol{x}, t) + C_i[f_1, \ldots, f_b], \qquad (19)$$

where $C_i[f]$ is the collision operator, a polynomial of degree b constructed explicitly out of all allowable n-body collisions, $2 \le n \le b$, among populations sitting on the *same* site $\boldsymbol{x}$ at time t. The above LBE has a simple interpretation: Particle population $f_i(\boldsymbol{x} + v_i, t+1)$ is equal to the post-collision $f_i'(\boldsymbol{x}, t)$ value advected from the "upper wind" position $\boldsymbol{x}$ at the previous time t. Here $f_i' \equiv f_i + C_i$. Thus C_i represents the change of the particle population by collisions. Compliance with mass and momentum conservation laws imposes the following constraints on the collision operator:

$$\sum_i C_i = 0, \quad \sum_i \boldsymbol{v}_i C_i = 0 \qquad (20)$$

If there is an energy degree of freedom, then we also have:

$$\sum_i \epsilon_i C_i = 0, \qquad (21)$$

where $\epsilon_i = \boldsymbol{v}_i^2/2$ for an ideal gas. As in continuum kinetic theory, this collision operator admits a detailed balance condition when all populations of different particle velocities are in equilibrium, $\{f_i = f_i^{\text{eq}}, \ \forall i\}$:

$$C_i[f^{\text{eq}}] = 0 \qquad (22)$$

Regardless of the detailed collision processes, the solution of Eq. (22) takes on a generic form dictated by the basic conservation laws,

$$f_i^{\text{eq}} = e^{-I_i} \qquad (23)$$

where $I_i = A + \mathbf{B} \cdot \boldsymbol{v}_i + C\epsilon_i$ is a linear combination of collisional invariants, while A and $\mathbf{B}$, in turn, are functions of local hydrodynamic quantities,

$$\rho(\boldsymbol{x}, t) = \sum_i f_i(\boldsymbol{x}, t) \qquad (24)$$

$$\rho\boldsymbol{u}(\boldsymbol{x}, t) = \sum_i \boldsymbol{v}_i f_i(\boldsymbol{x}, t) \qquad (25)$$

Once again, for systems with an energy degree of freedom, the total energy can be defined as,

$$\rho(DT + \boldsymbol{u}^2)/2 = \sum_i \epsilon_i f_i \qquad (26)$$

where D is the number of spatial dimensions and T can be interpreted as the temperature of the fluid.

The LB equation (19) obeys the so-called semi-detailed balance property for the collision operator as its Lattice Gas Cellular Automata predecessor (Frisch, Hasslacher and Pomeau, 1986; Frisch *et al.*, 1987). It can be shown that such a kind of collision operator admits a local H theorem with the following discrete Boltzmann entropy function, $h_{\text{B}}(\boldsymbol{x}, t) = \sum_i f_i(\boldsymbol{x}, t) \ln f_i(\boldsymbol{x}, t)$. In other words, an H theorem can be defined on each local lattice site, so that, without external disturbances or boundary influences, h_{B} is a non-increasing function of t satisfying the dynamics of C_i. Furthermore, the minimum value of $h_{\text{B}}(\boldsymbol{x}, t)$ is attained when the particle populations $\{f_i\}$ assume the equilibrium form given by (23), where A, $\mathbf{B}$ and C are constants determined by the values of mass, momentum and energy. Borrowing from the terminology of nonlinear dynamic systems, the existence of an H theorem ensures that the equilibrium distribution is not only a *fixed point* solution of (22) but also an *attractor* of the collisional dynamics. On the other hand, this is a weaker H theorem compared to its continuum counterpart, for the above does not include advection of particles among lattice sites according to (19). We will realize in a subsequent section that, unlike in continuum Boltzmann dynamics, the local H theorem in Lattice Gas Cellular Automata given above does *not* (except for the isothermal case, in which energy conservation is replaced by a constant temperature-like parameter) automatically lead to a global one, referred to as the global H-theorem (Frisch, Hasslacher and Pomeau, 1986; Frisch *et al.*, 1987, Chen, 1995; Chen, 1997). Generally the global H function is given by,

$$H(t) = \sum_{\boldsymbol{x}} h_{\text{B}}(\boldsymbol{x}, t).$$

Existence of a global H theorem in LB guarantees an asymptotically homogeneous spatial distribution of particles as time $t \to \infty$, and hence it provides a well-defined global hydrodynamic stability. As in standard kinetic theory, hydrodynamics concerns properties around the local equilibrium,

$$f_i = f_i^{\text{eq}} + f_i^{\text{ne}} \tag{27}$$

where the non-equilibrium component, f_i^{ne}, is supposed to scale like kf_i^{eq}, where the smallness parameter k, known as the Knudsen number, is the ratio of the particle mean free path to a typical hydrodynamic scale. Ordinary fluids feature Knudsen numbers below 0.01, see Chapman and Cowling, 1970.) The existence of a local H theorem makes a perturbation analysis purposeful since the dynamic system always approaches a defined equilibrium f_i^{eq} and evolves in the neighborhood of such a defined point. Perturbative treatment of the LBE up to second order in k (Chapman-Enskog procedure) is then expected to yield the hydrodynamic equations

$$\partial_t \rho + \partial_a \rho u_a = 0$$
$$\partial_t \rho u_a + \partial_b P_{ab} = 0 \tag{28}$$

where

$$P_{ab} \equiv \sum_i v_{ia} v_{ib} f_i^{\text{eq}} + \sum_i v_{ia} v_{ib} f_i^{\text{ne}} \tag{29}$$

$$= g\rho u_a u_b + P\delta_{ab} + \rho\nu[\partial_a u_b + \partial_b u_a - \frac{1}{D}(\partial_c u_c)\delta_{ab}]$$

is the momentum-flux tensor comprising both non-viscous and dissipative components, the latter being proportional to the fluid viscosity ν. In the above, P is the resulting pressure, and D is the dimensionality of a lattice. Note that the prefactor g in the advection term which signals a potential breaking of Galilean invariance whenever $g \neq 1$. On the other hand, since g depends only on the fluid density ρ, for incompressible flows in which the density is constant in space and time, Galilean invariance can be recovered by a simple rescaling of time, pressure and viscosity:

$$t' = gt, \quad \nu' = \nu/g, \quad P' = P/g$$

Clearly, even within the framework of incompressible flows, this rescaling does *not* extend to more general situations, such as multi-component or multi-phase flows.

A. The fully non-linear LBE

The fully non-linear LBE, eq. (19), was first proposed by McNamara and Zanetti (McNamara, Zanetti, 1988), who realized its potential for doing away with the statistical noise problem affecting Lattice Gas Cellular Automata simulations (Orszag, Yakhot, 1986, Succi, Santangelo, Benzi, 1989). All other weaknesses still remained. In general, the factor g is not equal to unity,

indicating a violation of Galilean invariance. Though a choice of sufficient lattice symmetry ensures a rotationally invariant form of P_{ab}, the resulting local equilibrium in typical Lattice Gas Cellular Automata collisions does not have a suitable functional form for achieving a correct Navier-Stokes hydrodynamics, which requires $g = 1$. Indeed, in order to obtain the correct form of the Navier-Stokes equation, the local equilibria must comply with a specific form as a function of the local hydrodynamic variables, ρ and $\boldsymbol{u}$, (S. Chen *et al.*, 1991; H. Chen, S. Chen and Matthaeus, 1992; Qian, d'Humieres and Lallemand, 1992).

In addition to incorrect hydrodynamics, Lattice Gas collisions have problems in attaining low viscosity. The fluid viscosity is approximately given by $\nu = 3Dlv_T$, where l is the particle mean-free path and v_T the typical particle thermal speed. In many problems, for instance turbulence, we are interested in very low-viscous flows, which means very short mean-free paths. On the other hand, short mean-free paths imply many collisions.

We are thus forced to consider as far as possible all allowable types of collisions among the set of discrete velocities. Unfortunately, it turns out that the full collision operator C_i involves an exponential barrier of the order of 2^b operations, in direct contradiction with the basic commitment to simplicity and computational efficiency of the method.

B. The LBE in scattering form

Building upon the idea that many-body collisions are not essential to achieve the correct hydrodynamic limit, Higuera and Jimenez (Higuera and Jimenez, 1989) realized that the collision operator can be reduced to a dramatically simpler two-body scattering expression:

$$C_i \to \sum_j A_{ij}[f_j - f_j^{\text{eq}}], \tag{30}$$

where the scattering matrix A_{ij} is basically the Jacobian of the fully non-linear operator C_i evaluated at the uniform equilibrium values $f_i = \rho/b$. The above expression turns a daunting 2^b complexity into a much more manageable b^2 one, thus opening the way to three-dimensional Lattice Boltzmann hydrodynamics. Of course, compliance with an H-theorem is no longer guaranteed because the local equilibrium is no longer the direct result of collisional dynamics.

In addition, since the scattering matrix A_{ij} is still related one-to-one to the underlying Lattice Gas Cellular Automata microdynamics, the corresponding Lattice Boltzmann equation shares the same limitations in terms of high viscosity, i.e., low Reynolds numbers.

C. The self-consistent LBE

This last limitation can be wiped out by a mere change in perspective. Instead of deriving the Navier-Stokes equation bottom-up (here bottom means the atomic level) from a truly N-body discrete dynamical system, we can *construct* it top-down from the sole requirement of compliance with the Navier-Stokes equations (Higuera, Succi and Benzi, 1989, Succi, Benzi, Higuera, 1991). The idea is to recognize that, as far as hydrodynamics is concerned, the key notions of scattering matrix and local equilibrium can be *prescribed* at the outset instead of being *derived* from an underlying (discrete) micro-dynamics. Mathematically, this amounts to prescribing the scattering matrix in spectral-form:

$$A_{ij} = \sum_{k=1}^{b} \lambda_k P_{ij}^{(k)}, \qquad (31)$$

where $P_{ij}^{(k)}$ projects along the k-th eigenvector in kinetic space and λ_k is the corresponding eigenvalue ($\lambda_k = 0$ for conserved quantities). Of particular interest is the leading non-zero eigenvalue, which is in direct control of the fluid viscosity $\nu \sim \lambda^{-1}$.

Once this point of view is endorsed, namely that local equilibria can be "freely" chosen within the conservation constraints, and that the scattering matrix can be selected a priori on the sole basis of conservation constraints, nothing prevents this Lattice Boltzmann equation from attaining as low viscosity as the lattice discreteness permits. Full contact with classical computational fluid dynamics is made (Chen H., S. Chen, W. Matthaeus, 1992). More importantly, the top-down approach, which proved so fruitful and influential for subsequent developments of LB theory, is established.

D. The lattice Bhatnagar-Gross-Krook equation

The LBE story has still one more nugget in store.

The scattering matrix can also be viewed as a multiple scale relaxation operator, one scale for each non-zero eigenvalue. Since we are basically interested in a single transport parameter, the fluid viscosity, a single eigenvalue should do. Indeed we can replace the full matrix A_{ij} with a single-parameter diagonal form $-\omega\delta_{ij}$, describing a single-time relaxation around a prescribed local equilibrium f_i^{eq}. In its simplest and by now most popular form, the relaxation-approximation corresponds to the following Lattice BGK (Bhatnagar-Gross-Krook) equation (Bhatnagar, Gross and Krook, 1954):

$$f_i(\boldsymbol{x}+\boldsymbol{v}_i, t+1) - f_i(\boldsymbol{x}, t) = -\omega[f_i(\boldsymbol{x}, t) - f_i^{\text{eq}}(\boldsymbol{x}, t)], \quad (32)$$

where exact Navier-Stokes hydrodynamics is obtained with the following choice of local-equilibrium form,

$$f_i^{\text{eq}} = w_i\rho\left\{1 + \frac{\boldsymbol{v}_i \cdot \boldsymbol{u}}{T} + \frac{(\boldsymbol{v}_i\boldsymbol{v}_i - v^2) : \boldsymbol{u}\boldsymbol{u}}{2T^2}\right\}. \qquad (33)$$

where the symbol : stands for tensor scalar product. In the above, w_i is a suitable lattice-dependent weighting factor, and the temperature $T = 1/3$ in typical isothermal lattice BGK models (S. Chen *et al.*, 1991; H. Chen, S. Chen and Matthaeus, 1992; Qian, d'Humieres and Lallemand, 1992; Chen, Teixeira and Molvig, 1997). Since temperature is frozen to a constant value, these lattices models should best be denoted as "a-thermal" rather than "iso-thermal". More comments on this delicate issue shall be presented later in this paper. For a thorough and beautiful discussion of the subtleties of lattice thermo-hydrodynamics, the reader is recommended to consult Rivet & Boon, Chapter IV.

It is readily recognized that this formulation leads to a Galilean invariant Navier-Stokes equation (up to terms of order $Mach^4$, where $Mach$ is the Mach number, namely the ratio of fluid to sound speed), for a fluid of viscosity $\nu \sim T/\omega$. The LBE scheme in relaxation form has met with significant success in the last decade in simulating a variety of fluid flows. Indeed, the lattice BGK equation and subsequent straightforward extensions to allow a variable Prandtl number (ratio of momentum to heat diffusivity) (Keizer, 1987, Chen et al 1997), represents the method of choice in the field. Very interesting variants, combining the best features of the Lattice Boltzmann equation in scattering form and Lattice BGK have also been developed (D'Humières, 1992).

A few years later it was shown that the Lattice BGK can be derived from the continuum Boltzmann BGK equation by a Grad-like moment expansion supplemented with numerical quadrature for the actual evaluation of the kinetic moments (He and Luo, 1997; Shan and He, 1998). Realizing such a connection might prove very useful for establishing new lattice BGK's starting from model continuum Boltzmann equations, hopefully including physics beyond the hydrodynamic level.

While focus on the conservation laws (hydrodynamic constraints) was the leit motif of all the aforementioned developments, compliance with the second thermodynamic principle, namely the existence of the H theorem, was somehow left in a subdued light by the top-down approach. That neglect had no serious consequences, because, thanks to a gracious smile from Lady Luck, being cavalier about an underlying H theorem proved very forgiving for *isothermal* LBE flows (the bulk of early LBE research) even at very low viscosities, where numerical stability is severely probed. By now, we have learned that this favorable behavior is due to the existence of an underlying H theorem, as we shall detail in the next section.

V. H THEOREM IN DISCRETE PHASE-SPACE

The H theorem is a milestone of non-equilibrium statistical mechanics, since it provides a conceptual link between the reversible laws of the microworld and the one-sided nature of macroscopic phenomena (Lebowitz, 1993;

Lieb, 2000). It is also a fundamental concept in computational physics, where compliance with an H theorem is often perceived as a byword for numerical stability (Perthame and Tadmor, 1991; Natalini, 2000; Junk and Klar, 2000). H-compliant Discrete-Velocity Boltzmann (DVB) equations have been known for a long time (Broadwell, 1964, Gatignol, 1965), but, as discussed previously, they are not meant to compete with Navier-Stokes solvers because their main focus is maximum likelyhood to the Boltzmann equation in the high-Knudsen regime. This leads to discrete collision operators which are just too complicated to serve as a practical tool for purely hydrodynamic purposes.

Computational complexity dissolves by using relaxation approximations, notably lattice BGK, and it is therefore imperative to explore the possibility of establishing H theorems for lattice BGK. Before plunging into this theme, a few reflections on the classical case are in order.

A. Reflections on the continuum case

The classical Boltzmann H theorem is so familiar that it is worthwhile to look at it from the perspective of modeling, in order to better understand what is actually lost and needs to be rearranged when going from the continuum to the Lattice Boltzmann case.

First, we find that the familiar local Maxwell distribution function (the "Maxwellian") minimizes the H function, $H = \int f \ln f \, dv$, as soon as the five hydrodynamic invariants (mass, momentum and energy), are fixed. Furthermore, we observe that all higher-order moments of the local Maxwellian distribution are just in the right form for the Chapman-Enskog expansion to deliver the Navier-Stokes equations. Backed with this information, we start looking for a kinetic model acting as a continuous-time constrained minimization process of this H, in such a way as to conserve the hydrodynamic moments. We readily find several such models: the Boltzmann equation itself, the BGK model, the diffusion equation, and so on. All of these models differ only in the way relaxation to the local equilibrium takes place; some of them do require explicit knowledge of the local Maxwellian (the BGK), some others don't. They all deliver the Navier-Stokes equation in the end, with the only differences among them occurring in the transport coefficients, whose evaluation is simple for the BGK and requires some (non-negligible) work for the Boltzmann equation. In all models the collision integral has the local Maxwellian as its zero point. The rate at which the H function decreases in time is just equal to the entropy production (we recall that entropy is the space integral of the $-H$ function) and entropy production becomes zero in the local Maxwell state. The local Maxwellian distribution is then characterized in three different but equivalent ways: *It is the minimum of H, it is the zero point of the collision integral, and it is the zero point of the entropy production.*

When moving to the lattice world the basic question to be addressed is: *how does the H theorem transform in the discrete-time case?*

The first good news is that *all velocities are in some finite range*, so that we can think of local equilibria for the given density and velocity alone, without necessarily including energy. In the (non-relativistic) continuum, energy *must* be included, for otherwise nothing would prevent integrals over velocities from diverging. The flip side is that since discrete speeds come in a very(!) finite number, the Boltzmann H function does *not* work: For any known lattice, a straightforward computation demonstrates that the local Maxwellian equilibrium does not imply correct expressions for the higher-order moments. On the other hand, a priori, there is a huge class of convex functions at our disposal, and in order to illustrate the idea of what local equilibria may look like in the lattice context, we shall present an example of a solvable lattice entropy, $H_{1/2} = \sum_{i=1}^{b} f_i \sqrt{f_i}$ [1]. For this entropy, the local equilibrium can be found explicitly (Karlin *et al.*, 1998)

$$f_i^{\text{eq}} = \frac{\rho}{b} \left[\frac{1}{2} \left(1 + \sqrt{1 - M^2} \right) + \frac{\boldsymbol{u} \cdot \boldsymbol{v}_i}{c_{\text{s}}^2} + \frac{(\boldsymbol{u} \cdot \boldsymbol{v}_i)^2}{2 c_{\text{s}}^4 \left(1 + \sqrt{1 - M^2} \right)} \right].$$
(34)

Here c_{s}^2 is the speed of sound squared, and $M^2 = u^2/c_{\text{s}}^2$ is the local Mach number squared. The above equilibrium is Galilean-invariant only in the limit of vanishing flow, $M \to 0$. At any finite flow speed, a quadratic (in the Mach number) anomaly is apparent. Because advection terms in the Navier-Stokes equations are also quadratic in velocity, such a rapid growth of anomalies rules out the use of the function $H_{1/2}$ for constructing the Lattice Boltzmann method. This is the typical situation of first-generation Lattice Gas and Lattice Boltzman models. Nevertheless, it is instructive to look at Eq. (34) and see how lattice equilibria differ from the local Maxwellian. Recall that the local Maxwellian is a well-defined function for all values of the average velocity. In contrast, the local equilibrium (34) is positive only for $M < 1$, and it does not exist as a real-valued function, for $M > 1$. This means that no collision mechanism is able to equilibrate the non-equilibrium deviations produced by the supersonic motion, and therefore no macroscopic dynamics for this regime can exist. This conveys an intriguing flavour of relativistic mechanics, which is after all not surprising since lattice molecules move at the lattice speed of light c equal to the maximal length of the lattice link.

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[1] This entropy function belongs to the class of Renyi (or Tsallis) entropies, $H_p = (f^{p+1} - f)/p$, with $p = 1/2$. This is a glorious class of functions of modern statistical physics, for it provides the stepping stone for the celebrated replica method in spin-glass theory, multifractal ideas and also non-extensive thermodynamics (Tsallis, 1988).

In order to proceed sensibly, three basic requirements must be faced:

- *Galilean invariance*

- *Realizability*

- *Solvability*

each of which we now discuss in some detail.

B. Galilean invariance

Galilean invariance requires kinetic equilibria to depend on the relative speed $\boldsymbol{v} - \boldsymbol{u}$ ("peculiar" speed) rather than on the absolute molecular speed $\boldsymbol{v}$ itself. In the continuum, this is ensured by the Maxwellian dependence, $\sim \exp\{-(\boldsymbol{v}-\boldsymbol{u})^2/v_T^2\}$, where $v_T \equiv \sqrt{2k_\mathrm{B}T/m}$ is the thermal speed, which sets the natural scale for molecular fluctuations around the fluid speed $\boldsymbol{u}$. In the Lattice Boltzmann setting, we have already committed ourselves to low Mach numbers and no compressibility effects. Therefore, it seems reasonable to proceed with expansion of the local Maxwellian around the global equilibrium ($\boldsymbol{u} = 0$). Since the Maxwellian is a transcendental function, large departures from global equilibrium require virtually an infinite number of terms of this expansion.

Terms that correspond to kinetic excitations on top of the uniform "ground state" are described by higher order polynomials in the velocity variable. Since a finite set of discrete speeds can only support a finite number of these excitations, breaking of Galilean invariance cannot be avoided. The above considerations suggest that Galilean invariance can be recouped to some order if local equilibria can be expressed in the form of finite-order *polynomials* of the flow speed.

The question is then whether suitable polynomials can be found that still comply with a discrete H theorem. The answer to this question appears to be negative (Wagner, 1998): There are no convex entropy functions whose local equilibria are the polynomials of the form used in the lattice BGK.

In analogy with lattice field theory, we shall call Galilean-invariant discrete entropies as *perfect*, in that they "hide" the underlying lattice discreteness. Are there perfect entropy functions for the Lattice Boltzmann method? At the time of this writing, no perfect lattice entropy is known, and most probably there is none, so that we are led to conclude that the Lattice Boltzmann method is not capable of reproducing the full properties of the continuum Boltzmann equation.

However, *quasi-perfect entropies*, namely entropies which are not affected by lattice discreteness (up to fourth order terms in the Mach number) have indeed been found by a customized, lattice-dependent procedure (Karlin, Ferrante and Öttinger, 1999). As an illustration, for a three-state one-dimensional lattice with $\boldsymbol{v}_0 = 0$ and $\boldsymbol{v}_{\mp 1} = \mp 1$, the following quasi-perfect Boltzmann-like H-function is identified:

$$H = f_0 \ln(f_0/4) + f_+ \ln f_+ + f_- \ln f_-. \qquad (35)$$

Given the fact that the Lattice Boltzmann equation is itself a second order approximation in the Mach number to the Navier-Stokes equations, these quasi-perfect entropies must be regarded as definitely adequate for hydrodynamic purposes.

The explicit form of the local equilibria corresponding to the quasi-perfect Boltzmann-like entropy functions is not known, in general. However, polynomial approximations can be found up to the relevant order in Mach number. These approximations coincide with those established earlier for the lattice BGK, and this now explains why the Lattice Boltzmann works in this case: These specific polynomial equilibria survived among other possible Galilean-compliant polynomials because they are computationally more stable than others, and it is precisely these polynomials which are supported by the quasi-perfect entropy functions. The existence of quasi-perfect lattice entropies achieves a formal compliance with the second law of thermodynamics and provides a strong incentive to pursue further development of the Lattice Boltzmann method based on the entropy maximization principle.

C. Realizability

Realizability is simply the condition that local equilibria resulting from an entropy maximization procedure be real-valued and between zero and one:

$$0 < f_i^\mathrm{eq} < 1 \qquad (36)$$

By itself, realizability is neither a *necessary* nor a *sufficient* condition for stability, although it generally helps stability (Renda et al, 1998). At any rate, it is a good pre-requisite, at least until we learn to deal sensibly with negative distribution functions.

It should be appreciated that gradient-driven departures from local equilibrium can violate the realizability constraints even if the local equilibria don't. Therefore the stability domain in kinetic space is by necessity a subset of the realizability domain. Manifestly, the polynomial nature of the discrete local equilibria is a potential danger to the realizability constraint, a danger which simply does not exist in the continuum.

Description of realizability domains on the lattice is a nontrivial problem with an interest of its own. In a recent work, Boghosian's et. al (2001) applied the powerful Fourier-Motzkin technique of linear programming to classify automatically the realizability domain associated with a given set of constraints.

This may help the systematic search for optimal lattice entropies.

D. Solvability

Solvability refers to the possibility of expressing local equilibria as explicit functions of the conserved hydrodynamic variables, i.e., density ρ and flow speed $\boldsymbol{u}$. This is very important since it permits one to explicitly recast kinetic theory in terms of an equivalent set of partial differential equations for space-time dependent continuum fields. Solvability has also a considerable practical impact on the efficiency of lattice BGK schemes, for it implies that local equilibria can be encoded once and for all as analytic functions of the hydrodynamic variables. Local equilibria resulting from non-solvable entropies must be recomputed numerically at each time step by iterative procedures and deprive lattice BGK of (part of) its simplicity and efficiency. A way out of this problem is to restore the Boltzmann-like collision operators which can be constructed from just the knowledge of the entropy. (We recall that even the single relaxation time property is not exclusively the property of the Bhatnagar-Gross-Krook equation). This has been done recently (Ansumali and Karlin, 2000).

E. Discrete-time effects and the mirage of zero-viscosity

Perhaps the most interesting feature of the discrete-time kinetics is that the H-theorem is no longer the same (qualitatively) as in the continuous-time case. The way the H-theorem features itself in the Discrete Velocity Models, where time is still continous, is basically the same as in the classical theory. When time is discrete, things change considerably.

The major distinction is that, in order to achieve interestingly low values of the transport coefficients, the lattice relaxation dynamics must proceed in artificially long (hence more effective) jumps going across the maximum entropy point (equilibrium), in a sort of two-sided *over-relaxation* process, which bears little resemblance to the smooth relaxational trajectory of the continuum case. The problem is best illustrated in geometrical terms (see Figure 4): If f is the set of populations at time t, then the collision operator gives the direction, $C(f)$, in the kinetic space in which the populations must be moved (these directions change at different lattice nodes). Let us consider populations $f + \beta C[f]$, where $\beta > 0$. When tracing the ray $f + \beta C[f]$, starting with $\beta = 0$, we see that the function H is decreasing (because the classical entropy production, $-\sum_i C_i[f]\partial H/\partial f_i$, is positive), then comes to the minimum at some β', then starts increasing which would not be allowed if time were continous. In discrete time we can still safely place the populations in the increasing branch until $H(f + \beta C[f]) < H(f))$, and finally come to a value β^* where the entropy just equals the initial value $H(f)$. Formally, the condition:

$$H(f) = H(f + \beta^* C[f]), \qquad (37)$$

sets the limit for the over-relaxation. It has been shown (Karlin et al, 1998; Karlin, Ferrante and Öttinger, 1999; Boghosian et al, 2001) that this estimate reduces to the so-called linear stability interval, $0 < \omega < 2$ for the lattice BGK, required by the positivity of transport coefficients, as soon as the state is close to the local equilibrium. Recall that in the classical continuous-time kinetic theory, positivity of transport coefficients is ultimately related to positivity of the local entropy production. *It is remarkable that the lattice local H-theorem establishes the same result for the discrete-time case since positivity of transport coefficients follows now from the estimate (37).* In other words, it is clear that in the over-relaxation scenario there is no guarantee that the post-collisional state generally attains a smaller H-value than the pre-collisional state. This is controlled by the global shape of the entropy function *far* from equilibrium. In fact, if the value of ω is too large, the end-point may run into a lower entropy state, or some populations may even become negative. Both such outcomes set the stage for the type of kinetic instabilities hindering the application of the Lattice Boltzmann method to very low viscous, high Reynolds flows.

This discussion shows that the "mirage" of zero-viscosity, so crucial for turbulence studies, falls within the general problem of finding a systematic formulation of the dynamics of dissipative systems *far* from equilibrium (Prigogine, 1962; Ruelle, 1999).

With the quasi-perfect entropy at hand, we make full contact with the second law of thermodynamics, and establish the "smallest" Boltzmann system: It has the properly defined local equilibrium, the H theorem, and the correct hydrodynamics to the minimal required order of approximation.

The discrete-time H-theorem suggests the possibility of increasing stability at low viscosity by implementing the estimate (37). In fact, Lattice Boltzmann schemes endowed with quasi-perfect entropies, and with the entropy estimate (37) implemented, are generally found to exhibit better numerical stability. Typical instabilities associated with the lack of the H-theorem are shown in Figures 5 and 6. In Figure 5 we show the density profile for a one-dimensional front in a shock tube at time $t = 500$ (in lattice units) for the Lattice Boltzmann with entropy function (Ansumali and Karlin, 2000) (top picture, labelled ELBM), the Lattice BGK model based on the polynomial ansatz of Qian, d'Humieres and Lallemand (1992), (middle picture labelled LBGK), and the Lattice Boltzmann model by Qian, D'Humières and Lallemand, 1991, (bottom figure, labelled LBE). The viscosity is set to $\nu = 10^{-1}/3$. From Figure 5, we notice that, although LBE is producing the most accurate solution almost everywhere, only ELBM is free of non-physical oscillations (known as "Gibbs phenomenon" in numerical analysis), typical of non-entropic numerical schemes and often a precursor of numerical instabilities. Indeed, a minor decrease of the viscosity is found to disrupt the stability of the LBE simulation. By further decreasing the viscosity,

LBGK also becomes unstable, whereas ELBM does not. On the other hand, the better ELBM stability comes at the expense of some oversmoothing of the fronts, as it is visible by comparison with the thin line (top figure) giving the exact solution. The Figure 6, which shows the corresponding velocity profile, tells essentially the same story: the long-standing conflict between stability and numerical diffusion, a sort of "numerical uncertainity principle" (Boris, 1989). For very recent improvements of the ELBM approach in the direction of decoupling the conflicting issues of numerical stability and accuracy, see Ansumali and Karlin, (2002a, 2002b).

F. Over-constrained equilibria

We emphasize that local equilibria of the quasi-perfect entropy are "classical": They minimize the entropy under constraints provided by the locally conserved fields, whereas the desired conditions for the non-conserved fields (the local equilibrium momentum flux tensor in the above consideration) follow from this solution.

What happens if the set of constraints is enlarged in such a way as to include higher-order moments?

It should be noted that this is a rather unconventional move since the momentum flux tensor does *not* originate from a microscopic collisional invariant. This move is motivated by the fact that the search for good entropies cannot keep up with the needs raised by various Lattice Boltzmann models: while it is rather easy to establish the set of constraints on the equilibrium, it is much less easy, even approximately, to find an entropy whose maximum, under fixed conserved fields, would also imply the rest of the constraints which do *not* come from the conservation laws. For this reason, one could try to force the solution, proceeding with any entropy of choice, but with more constraints. For instance, it is clear that minimizers of convex functions under constraints,

$$\sum_i f_i^{\text{eq}}[1, \boldsymbol{v}_i, \boldsymbol{v}_i\boldsymbol{v}_i] = \rho[1, \boldsymbol{u}, (P/\rho)\boldsymbol{1} + \boldsymbol{u}\boldsymbol{u}], \qquad (38)$$

are Galilean-invariant *by construction* since they encode the correct equilibrium form of the momentum-flux tensor right at the outset. (Any further requirements on the equilibrium can be added in the same manner.) The picture is clear: for D spatial dimensions, the above set of constraints generates $N_c = 1 + D + D(D+1)/2 = (D+1)(D+2)/2$ equations for the set of N_c Lagrange multipliers $A, \boldsymbol{B}, \boldsymbol{C}$ forming the *quasi*-invariant $Q_i = A + \boldsymbol{B} \cdot \boldsymbol{v}_i + \boldsymbol{C} : \boldsymbol{v}_i\boldsymbol{v}_i$, where the symbol ":" stands for the tensor scalar product. These equations are generally non-linear (if the entropy function is not quadratic in the populations) and consequently very hard to solve– if solvable at all–analytically in order to deliver closed expressions for the overconstrained local equilibrium as a function of the hydrodynamic fields. But even this is not the main drawback. More importantly, such over-constrained equilibria confine the domain of the phase space where the entropy production is positive to rather "thin" subsets (Karlin and Succi, 1998). This explains why the Lattice Boltzmann method offers less stability in such cases than non-isothermal hydrodynamics, where constructions of the equilibria have been focused mostly on satisfying the conservation constraints regardless of their origin.

VI. DIRECTIONS FOR FUTURE RESEARCH

To date, there are still several directions where the Lattice Boltzmann theory calls for substantial progress and upgrades. Here, we shall briefly touch upon just two major streams of development:

- *Thermal flows*

- *Non-ideal fluids*

In a nutshell, the problem is to guarantee a sufficient lattice symmetry to ensure the correct evolution of *both* kinetic and potential energy, without loosing numerical stability. This is fairly non-trivial, since it involves control on higher-order local kinetic momenta, such as the heat flux, as well as on non-local information due to potential energy interactions.

As a further prospective area of future development we mention

- *Quantum systems*

for which much less has been done to date.

A. Thermal LBE's

Thermal field theories are notoriously hard (Umezawa, 1993), and Lattice Boltzmann theory is no exception. To date, isothermal, or better said, *athermal* LB systems[2] are way better understood than their thermal counterparts. The correct treatment of energy degrees of freedom in a lattice still poses a number of basic questions.

Energy dynamics in Lattice Boltzmann models is accounted for by enlarging the set of discrete speeds, 26 being the number of kinetic moments to be matched by the set of discrete speeds. Early experiments (McNamara, Garcia and Alder, 1995) showed that thermo-hydrodynamic LBE's exhibit a high degree of *molecular individualism*; errors in higher order moments seem to penetrate down into the low-order thermo-hydrodynamic

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[2] Since LBE is based on a collection of mono-energetic beams $\delta(\boldsymbol{v} - \boldsymbol{v}_i)$ in velocity space, the discrete LB distribution function is more appropriately classified as a zero-temperature system. We shall nonetheless stick to the more intuitive, if less rigorous, notation of *isothermal* schemes, to indicate that temperature is not a dynamic variable.

manifold. Similar type of difficulties have been recognized since long also in continuum kinetic theory (Lewis, 1967).

Despite significant progress, starting with the work of Alexander et al (Alexander, Chen and Sterling, 1993) thermal LBE's remain less robust than their isothermal counterparts.

Thermal LBE's might be subject to a sort of numerical instability similar to the one affecting high-order finite difference schemes: due to the presence of high-energy particles, large-set of discrete speeds give rise to high-order dispersion relations, which in turn might develop spurious branches and unphysical solutions.

This points even more strongly to the importance of a lattice H theorem. Again, a qualitative effect of lattice discreteness enters the scene. In the continuum, the local H theorem (positive entropy production due to collisions alone) does *not* explicitly involve transition probabilities from pre- to post-collisional states, and the detailed balance among different states are determined only by particle distributions with no other weighting factors. As a result, the H theorem is unaffected by particle advection since entropy is passively transported along collision-free trajectories. *Consequently the local H theorem automatically implies the overall H theorem (or "global H theorem").* In the discrete case, however, *the H theorem does depend explicitly on transition probabilities*, which are functions of local collisional invariants (Molvig *et al.*, 1988; Teixeira, 1992; Chen, Teixeira and Molvig, 1997; Chen, 1995; Chen, 1997; Chen and Teixeira, 2000). This is necessary to ensure that the resulting local equilibrium has a suitable form for producing correct thermo-hydrodynamic equations satisfying Galilean invariance (Frisch, Hasslacher and Pomeau, 1986; Frisch *et al.*, 1987). The condition for achieving the correct thermohydrodynamics requires the equilibrium form given by Chen (1995), namely an expansion up to $O(u^3)$ of a discrete local Maxwellian:

$$f_i^{\text{eq}} = \rho g_i(T) e^{\epsilon_i/T} exp[-(\boldsymbol{v}_i - \boldsymbol{u})^2/2T] \qquad (39)$$

where T is the local hydrodynamic temperature,

$$\rho(DT + \boldsymbol{u}^2)/2 = \sum_i \epsilon_i f_i$$

This form can be realized via explicit lattice gas particle collisions involving transition probabilities of $g_i(T)$ (Chen, 1995; Chen, 1997). On the other hand, as per the discussion above, relaxation to a given local equilibrium needs not proceed through explicit collisions. It can be shown that (39) admits a local H function of the form:

$$h = \sum_i f_i ln(f_i/g_i) \qquad (40)$$

The global H function may be simply defined as

$$H = \sum_{\boldsymbol{x}} h(\boldsymbol{x}).$$

Because of its explicit dependence on transition probabilities, the H value changes during the LBE advection phase, the result being that as particles hop in discrete steps from one lattice site to another, the values of the H function change *ahead* of the transition probabilities (which change during advection). This hinders translational invariance and sets the stage for a spontaneous symmetry breaking of the H theorem with no counterpart in the continuum. Since the transition probabilities, g_i, are functions of local hydrodynamic temperature, their value changes from place to place as particles move around the lattice. The violation of the global H theorem manifests itself whenever the temperature field acquires a spatial dependence. On the other hand, though the transition probabilities are not unity, they become constants in the isothermal LB models, which explains why the above problem disappears for isothermal LB models. This essential difference between thermal and isothermal lattice models lies at the heart of the significantly better stability of the latter.

In summary, aside from low-Mach number expansions in the usual lattice BGK, isothermal models have been shown to possess an H theorem (i.e., global H theorem), while thermal models have not. Proving an H theorem and subsequently constructing an H theorem obeying the Lattice Boltzmann process for thermal models remains an outstanding problem in Lattice Boltzmann research.

B. LBE for non-ideal fluids

Lattice Boltzmann schemes for multiphase, multicomponent fluid flows are often heralded as a most promising territory for LBE research. Indeed, there exist several extensions of the plain Lattice Boltzmann schemes for hydrodynamics which are able to include non-ideal gas effects (intermolecular interactions) (Shan and Chen, 1993, 1994 Swift, Osborne and Yeomans, 1995, Luo 1998, 2000). Most of these models can be cast in the form of a generalized LBE where the right-hand side is enriched with a (*self-consistent*) source term F_i:

$$f_i(\boldsymbol{x} + \boldsymbol{v}_i, t+1) - f_i(\boldsymbol{x}, t) = -\omega[f_i - f_i^{\text{eq}}](\boldsymbol{x}, t) + F_i \quad (41)$$

Formally, F_i is the lattice version of the one-body self-consistent force (vector notation relaxed for simplicity):

$$F(1)f(1) = \int f_{12}(1,2)F_{12}(1,2)d2 \qquad (42)$$

where f_{12} is the two-body distribution function, F_{12} the two-body force, and $1, 2$ stand for six-dimensional phase-space coordinates. Since the two-body distribution is likely to be computationally intractable, Lattice Boltzmann research moved in the direction of a *dynamic lattice density functional theory* (Hansen and Mc Donald, 1986), in which the effective force $F(1)$ is represented by a semi-empirical functional of the macroscopic state of

the system, namely density, flow fields and their derivatives:

$$F(1) = -\nabla\Psi[\rho, \boldsymbol{u}, ...] \qquad (43)$$

These schemes have been validated for a series of test cases and complex flows applications, yielding fairly interesting results (as an illustration, see Figure 7).

However, none of them has been proved to admit an underlying H theorem (Rothman, Keller and Gunstensen, 1991; Shan and Chen, 1993; Shan and Chen, 1994; Swift, Orlandini and Yeomans, 1995). This is in part due to the fact that equilibrium distribution functions depend on non-local properties. In other words, non-local information determines the transition probabilities. Consequently, similar to the problem encountered in the thermal LB models, advection changes globally defined quantities such as a H function. Another major theoretical issue is the nature of the hydrodynamic limit near thin-interfaces where the low-Knudsen assumption behind LBE is seriously challenged (a similar issue arises in the formulation of LBE-based renormalization group treatments of fluid turbulence (Chen, Succi, Orszag, 1999)).

Finally, as indicated earlier in this paper, the properties of the H theorem in the presence of a self-consistent force, are much less understood even in the continuum, Even though a global entropy production in the sense of decreasing H still exists in continuum Boltzmann, the issue of convexity and uniqueness of a minimum point becomes moot because the local condition $dH/dt < 0$ no longer guarantees that collisional dynamics will attain a *global* minimum. Besides serving the purpose of formulating better Lattice Boltzmann models, we believe this can be regarded as a fundamental research topic of general interest in non-equilibrium statistical mechanics (Lebowitz, 1999).

C. LBE for quantum systems

To date, Lattice Boltzmann research is largely dominated by non-quantum physics applications. Nonetheless, LBE can and has indeed been extended to (simple) cases of quantum mechanical motion, typically in the form of the non-relativistic Schroedinger equation (Succi and Benzi, 1993, Succi 1996, Meyer 1997, Boghosian and Taylor 1997). The stepping stone to the quantum Lattice Boltzmann equation is the identification of the four-spinor wave function Ψ_i obeying the quantum relativistic Dirac equation with a *complex* discrete distribution function. By writing the Dirac equation as a complex Lattice Boltzmann equation, it can be shown that the non-relativistic limit taking the Dirac equation into the Schroedinger equation is formally analogous to the adiabatic limit yielding hydrodynamics from the Lattice Boltzmann equation.

The proof proceeds by writing the Dirac equation (in one dimension for simplicity) for a relativistic particle of rest mass m as two coupled LBE's for a pair of complex upward and downward propagating spinors $u(z,t)$ and $d(z,t)$ respectively:

$$\partial_t u + \partial_z u = \omega_c d \qquad (44)$$
$$\partial_t d - \partial_z d = -\omega_c u$$

where $\omega_c = mc^2/\hbar$ is the Compton frequency of a material particle. By applying the unitary transformation:

$$\phi^{\pm} = \frac{1}{\sqrt{2}}(u \pm id)\, e^{i\omega_c t}$$

the above set of equations takes the following hydrodynamic form:

$$\partial_t \phi^+ + \partial_z \phi^- = 0 \qquad (45)$$
$$\partial_t \phi^- - \partial_z \phi^+ = 2i\omega_c u$$

From these equations it is apparent that the "slow" (hydrodynamic) symmetric mode is conserved, whereas the "fast" antisymmetric mode oscillates with a doubled frequency $2\omega_c$. It is now readily checked that the adiabatic assumption:

$$|\partial_t \phi^-| << |2i\omega_c \phi^-|$$

delivers precisely the Schroedinger equation for a free-particle of mass m. Since the adiabatic approximation involves an imaginary frequency, unlike the classical case, the hydrodynamic branch (i.e., the Schroedinger equation) remains time-reversible. This reversibility is somehow weaker than for the Dirac equation since it only applies to real time, whereas the Dirac equation is reversible in both real and imaginary time. Interesting connections to a quantum H-theorem might arise in the framework of the N-body quantum Lattice Boltzmann equation, a totally unexplored issue to the best of our knowledge.

The quantum LBE can be turned into a practical numerical scheme for the non-relativistic Schroedinger equation as well as for relativistic wave mechanics (Succi, 2002). It might also be suitable to quantum computing paradigms.

Saying that quantum LBE is a major issue of future Lattice Boltzmann research is probably an overstatement. Still, owing to the growing interest in quantum computing, the subject might be worth some attention in the years to come.

VII. CONCLUSIONS

These considerations complete the description of the Lattice Boltzmann method for isothermal Navier-Stokes equations as a self-contained kinetic theory admitting a proper H theorem. The corresponding theory for fully thermo-hydrodynamic LBE's is still in its infancy. Not only is further understanding of this subject crucial to the formulation of more stable numerical algorithms, but

it might also stimulate new insights into fundamental physical questions involving temperature dynamics and non-local intermolecular interactions in discrete dynamical systems.

VIII. ACKNOWLEDGMENTS

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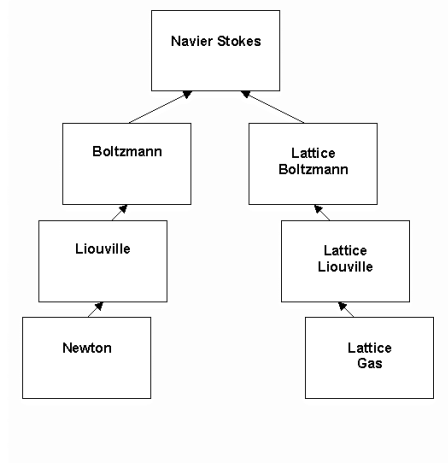[83] Zhang, R., S. Chen, and G. Doolen, 1999, J. Comp. Phys. **152**, 642.

FIG. 1 The BBGKY hierarchy and its lattice analogue. Lack of microscopic detail becomes less and less relevant as one proceeds upwards along the hierarchy (from Succi, (2001)).
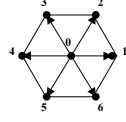
FIG. 2 The hexagonal lattice of the Frisch-Hasslacher-Pomeau cellular automaton. Particles move along the six discrete links and meet at lattice nodes where they interact according to mass and momentum-conserving collision rules.
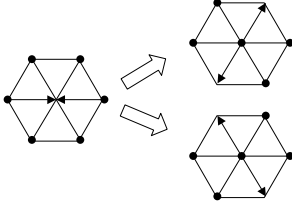
FIG. 3 A typical collision in the Frisch-Hasslacher-Pomeau cellular automaton. Both post-collisional outcomes (right) are equally probable. The left hand hexagon shows two particles initially at 9 o'clock and 3 o'clock moving in one time step to the central site. In the next time step, indicated by the hexagons on the right, their collision (conserving energy and momentum) results in the particles occupying the sites at 11 o'clock and 5 o'clock or 1 o'clock and 7 o'clock. They could return to their initial locations at 9 o'clock and 3 o'clock but this event is ruled out since it would not produce any observable effect since the particles are indistinguishable.
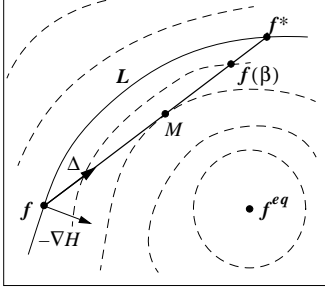
FIG. 4 Collisional relaxation procedure. Curves represent entropy levels, surrounding the local equilibrium f^{eq}. The solid curve L is the entropy level with the value $H(f) = H(f^*)$, where f is the initial, and f^* is the conjugate population. The vector $\boldsymbol{\Delta}$ represents the collision integral, the sharp angle between $\boldsymbol{\Delta}$ and the vector $-\boldsymbol{\nabla}H$ reflects the entropy production inequality. The point M is the minimum entropy state on the segment $[f, f^*]$ The result of the collision update is represented by the point $f(\beta)$. The choice of β shown corresponds to the "overrelaxation": $H(f(\beta)) > H(M)$ but $H(f(\beta)) < H(f)$. The particular case of the BGK collision (not shown) would be represented by a vector $\boldsymbol{\Delta}_{\mathrm{BGK}}$, pointing from f towards f^{eq}, in which case $M = f^{\mathrm{eq}}$.
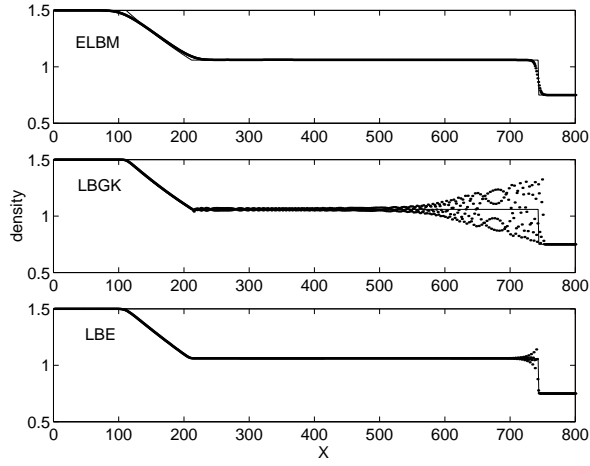
FIG. 5 Evolution of a one-dimensional front in a shock tube. Density profile (dimensionless lattice units) is shown at $t = 500$ for viscosity $\nu = 3.3333 \times 10^{-2}$. The figure compares three Lattice Boltzmann algorithms on the lattice with 800 nodes. Thin line: Exact solution at zero viscosity. Solid circles: Simulation. ELBM: The Lattice Boltzmann method based on the entropy function (from Ansumali and Karlin (2000)). LBGK: The Lattice BGK algorithm based on the polynomial ansatz of Qian, d'Humières and Lallemand (1992). LBE: The Lattice Boltzmann model of Qian, d'Humières and Lallemand (1991). The value of viscosity is taken close to the instability of the LBE.
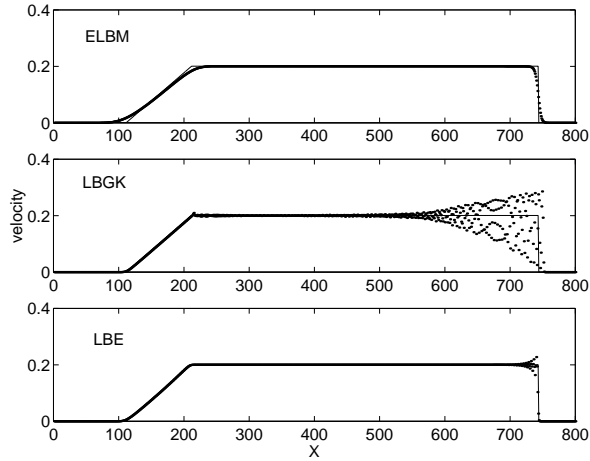
FIG. 6 Velocity profile in the one-dimensional shock tube benchmark. Simulation setup and notation are the same as in Figure 5
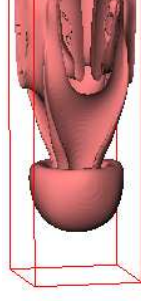
FIG. 7 A typical fluid interface exhibiting a single-mode Rayleigh-Taylor instability associated with a heavy fluid sitting on top of a light one. The density ratio of heavy and light fluids is 3. $Re = (gL)^{1/2}L/\nu = 1024$, $t/T_0 = 3.5$ $(T_0 = L/(gL)^{1/2})$, g being the gravitational acceleration driving the instability and L the box size. Periodic boundary conditions are used in horizontal directions and no slip boundary conditions are used in vertical directions (from Zhang, Chen and Doolen (1999), courtesy of Raoyang Zhang).